Ethyl lactate

97-64-3 | DTXSID6029127

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 19.1 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.63e-01

Confidence level: 5.94e-01

Nearest Neighbors from the Training Set

Image not found
1-Methoxy-2-propyl acetate
Measured: 2.29
Predicted: 7.33

Image not found
1,2-Diethylhydrazine
Measured: 15.1
Predicted: 14.1

Image not found
3-Pyridinecarbonitrile
Measured: 36.3
Predicted: 25.0

Image not found
2-(Pyridin-2-yl)ethanol
Measured: 28.2
Predicted: 35.9

Image not found
6-Methyl-2-thiouracil
Measured: 138
Predicted: 99.5